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IMPROVED TRADITIONAL ROSENBROCK–WANNER METHODS FOR STIFF ODES AND DAES



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Improved traditional Rosenbrock–Wanner methods for stiff ODEs and DAEs

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Abstract

Rosenbrock–Wanner methods usually have order reduction if they are applied on stiff ordinary differential or differential algebraic equations. Therefore in several papers further order conditions are derived to reduce this effect. In [13] the example of Prothero and Robinson is analysed to find further order conditions. In this paper we consider traditional ROW methods like ROS3P [7], ROS3PL [6], and RODASP [18] and modify these methods such that these further order conditions are satisfied. Numerical examples show the advantages of the new methods.

Keywords: ODEs, order reduction, ROW methods

1 Introduction

In the simulation of stiff ODEs or differential algebraic equations, the Runge–Kutta method seems to be a good choice since this class of methods contains explicit and implicit methods. Explicit methods may have the disadvantage that very small time step sizes have to be used to get a stable numerical result, and implicit methods need the solution of non-linear systems. A good compromise are linear implicit Runge–Kutta methods, so-called Rosenbrock–Wanner (ROW) methods which only need the solution of linear systems.

It is well known that an order reduction phenomenon can be observed if one-step methods are applied on stiff ODEs, or differential algebraic equations [2, 19]. Ostermann and Roche prove in [9] that implicit Runge–Kutta methods may have a fractional order of convergence for general linear ODEs. Similar results are presented for Rosenbrock–Wanner methods in [10]. Ostermann and Roche derive further order conditions for Rosenbrock–Wanner methods to reduce order reduction, since ROW methods have only stage order 1. For example, in [7] and [15] Rosenbrock–Wanner methods are derived which satisfy the order conditions from Ostermann and Roche [10] and which have almost no order reduction if they are applied on stiff ODEs, such as the Prothero–Robinson example or the semi-discretised Navier-Stokes equations [15, 14, 3, 4]. In [16] a different approach can be found for reducing the order reduction. An ROW method satisfying the order conditions derived by Scholz [16] is the RODASP method from Steinebach [18].

One well known example of a stiff ODE is the example of Prothero and Robinson [11]. In the book of Hairer and Wanner [2] the order reduction phenomenon is discussed for fully implicit Runge–Kutta methods. An analysis for diagonally implicit Runge–Kutta methods and Rosenbrock–Wanner methods can be found in [13]. In this paper new order conditions are derived which are a generalisation of the conditions from Ostermann and Roche [10] and Lubich and Ostermann [8]. The method ROS34PWR (see [12]) is an extension of method ROS34PW2 (see [15]) and satisfies the new conditions. This method is more effective than the old one, as numerical experiments show.

In this paper we consider some well known ROW methods such as ROSP [7], ROS3PL [6], RODASP [18] and ROS3Pw [15]. We will replace the old conditions from [10, 8] or from [16] (for the RODASP method) with the new order conditions. We will see that the number of internal stages does not increase. Numerical results show that the new methods are more effective.

2 Rosenbrock–Wanner methods

We start our considerations with an ODE of the form

$$\dot{\mathbf{u}} = \mathbf{F}(t, \mathbf{u}), \quad \mathbf{u}(0) = \mathbf{u}_0. \quad (1)$$

A Rosenbrock–Wanner–method (ROW method) with s internal stages can be formulated by

$$\mathbf{k}_i = \mathbf{F}\left(t_m + \alpha_i \tau_m, \tilde{\mathbf{U}}_i\right) + \tau_m J \sum_{j=1}^i \gamma_{ij} \mathbf{k}_j + \tau_m \gamma_i \dot{\mathbf{F}}(t_m, \mathbf{u}_m), \quad (2)$$

$$\tilde{\mathbf{U}}_i = \mathbf{u}_m + \tau_m \sum_{j=1}^{i-1} a_{ij} \mathbf{k}_j, \quad i = 1, \dots, s,$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau_m \sum_{i=1}^s b_i \mathbf{k}_i, \quad (3)$$

where $J := \partial_{\mathbf{u}} \mathbf{F}(t_m, \mathbf{u}_m)$ is the Jacobian of \mathbf{F} w.r.t. \mathbf{u} , α_{ij} , γ_{ij} , b_i are the parameters of the method,

$$\alpha_i := \sum_{j=1}^{i-1} \alpha_{ij}, \quad \gamma_i := \sum_{j=1}^{i-1} \gamma_{ij}, \quad \gamma := \gamma_{ii} > 0, \quad i = 1, \dots, s.$$

If the parameters α_{ij} , γ_{ij} , and b_i are chosen appropriately, a sufficient consistency order can be obtained. A derivation of these conditions with Butcher series can be found in [2]. Here we only summarize the conditions up to order 4:

$$\left\{ \begin{array}{ll} \text{(A1)} & \sum_{i=1}^s b_i = 1 \\ \text{(A2)} & \sum_{i=1}^s b_i \beta_i = \frac{1}{2} - \gamma \\ \text{(A3a)} & \sum_{i=1}^s b_i \alpha_i^2 = \frac{1}{3} \\ \text{(A3b)} & \sum_{i,j=1}^s b_i \beta_{ij} \beta_j = \frac{1}{6} - \gamma + \gamma^2 \\ \text{(A4a)} & \sum_{i=1}^s b_i \alpha_i^3 = \frac{1}{4} \\ \text{(A4b)} & \sum_{i,j=1}^s b_i \alpha_i \beta_{ij} \beta_j = \frac{1}{8} - \gamma/3 \\ \text{(A4c)} & \sum_{i,j=1}^s b_i \beta_{ij} \alpha_j^2 = \frac{1}{12} - \gamma/3 \\ \text{(A4d)} & \sum_{i,j,k=1}^s b_i \beta_{ij} \beta_{jk} \beta_k = \frac{1}{24} - \frac{1}{2} \gamma + \frac{3}{2} \gamma^2 - \gamma^3 \end{array} \right., \quad (4)$$

where we use the abbreviations $\beta_{ij} := \alpha_{ij} + \gamma_{ij}$ and $\beta_i := \sum_{j=1}^{i-1} \beta_{ij}$. Additional consistency conditions arise if J is only an approximation to

$\partial_{\mathbf{u}}\mathbf{F}(t_m, \mathbf{u}_m)$, or if J is an arbitrary matrix. This class of methods is called *W-methods*, [19]. The order conditions up to order 3 read as (see [19], [2], and [17]):

$$\begin{aligned} \text{(B2)} \quad \sum_{i=1}^s b_i \alpha_i &= \frac{1}{2} \\ \text{(C3a)} \quad \sum_{i,j=1}^s b_i \alpha_{ij} \alpha_j &= \frac{1}{6} \\ \text{(C3b)} \quad \sum_{i,j=1}^s b_i \alpha_{ij} \beta_j &= \frac{1}{6} - \frac{\gamma}{2} \\ \text{(C3c)} \quad \sum_{i,j=1}^s b_i \beta_{ij} \alpha_j &= \frac{1}{6} - \frac{\gamma}{2} \end{aligned} \quad (5)$$

The ROW method (2)–(3) requires the solution of s linear systems of equations with the same matrix $I - \gamma \tau_m J$. The right hand side of the i -th linear system of equations depends on the solutions of the first to the $(i-1)$ -st system. Thus, a main difference of ROW methods to implicit methods is that it is not necessary to solve a non-linear system of equations in each discrete time but only a fixed number of linear systems of equations.

If ROW methods are applied on semidiscretised parabolic problems they usually have order reduction. Therefore a ROW method should satisfy further order conditions. In this paper we follow the theory from [13] and consider the following conditions

$$\mathbf{b}^\top B^{-1} \boldsymbol{\alpha}^k = 1, \quad k = 2, \dots, p, \quad (6)$$

$$\mathbf{b}^\top B^{-(l+1)} \frac{1}{k-l} \boldsymbol{\alpha}^{k-l} = \mathbf{b}^\top B^{-l} [\boldsymbol{\alpha}^{k-l-1} + \gamma \delta_{k-l-1,1}], \quad (7)$$

for $l = 1, \dots, k-2$ and $k = 1, \dots, p+1$, where $\mathbf{b} = (b_1, \dots, b_s)^\top$, $B = (\beta)_{i,j=1}^s$, $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_s)^\top$, $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_s)^\top$, and δ_{ij} is the usual Kronecker product.

ROW methods allow an easy implementation of an adaptive time step length control, if the ROW method is of order $p \geq 2$. An adaptive time step control employs a second ROW method which has the coefficients a_{ij} , \hat{b}_i and c_i , $i, j = 1, \dots, s$, and order $p-1$. The solution of the second method at t_{m+1} is given by

$$\hat{\mathbf{u}}_{m+1} = \mathbf{u}_m + \sum_{i=1}^s \hat{b}_i \mathbf{k}_i.$$

Now, the next time step τ_{m+1} is proposed to be

$$\tau_{m+1} = \rho \frac{\tau_m^2}{\tau_{m-1}} \left(\frac{TOL \cdot r_m}{r_{m+1}^2} \right)^{1/p}, \quad (8)$$

where $\rho \in (0, 1]$ is a safety factor, $TOL > 0$ is a given tolerance and

$$r_{m+1} := \|\mathbf{u}_{m+1} - \hat{\mathbf{u}}_{m+1}\|. \quad (9)$$

This step size selection rule is called PI-controller and going back to Gustafsson et al. [1]. For details on the numerical error and the implementation of automatic step length control we refer to [2, 5].

3 Improvement of traditional ROW methods

3.1 The ROS3P method

First we consider the ROS3P method from Lang and Verwer [7]. It is a strongly A-stable scheme of order 3 with 3 internal stages. The method satisfies the order condition (A1), (A2), (A3a), and (A3b) and the conditions from Lubich and Ostermann [8]. We replace the second ones by the conditions (6) for $k = 2, 3$ and the condition (7) for $k = 3, 4$ and $l = 1, \dots, k - 2$. Then we have the following equations for the coefficients of the ROW method:

$$b_1 + b_2 + b_3 = 1, \quad (10)$$

$$b_2\beta_2 + b_3\beta_3 = \frac{1}{2} - \gamma, \quad (11)$$

$$b_2\alpha_2^2 + b_3\alpha_3^2 = \frac{1}{3}, \quad (12)$$

$$b_3\beta_{32}\beta_2 = \frac{1}{6} - \gamma + \gamma^2, \quad (13)$$

$$b_3\beta_{32}\alpha_2^2 = \frac{\gamma}{3} - \gamma^2, \quad (14)$$

$$\gamma(b_2\alpha_2^3 + b_3\alpha_3^3) - b_3\beta_{32}\alpha_2^3 = \gamma^2, \quad (15)$$

$$2b_3\beta_{32}\alpha_2^2 = \frac{\gamma}{3} - 2\gamma^3, \quad (16)$$

$$\gamma(b_2\alpha_2^3 + b_3\alpha_3^3) - 2b_3\beta_{32}\alpha_2^3 = 3\gamma^3, \quad (17)$$

$$b_3\beta_{32}\beta_2 = -2\gamma^2 + 2\gamma - \frac{1}{3}. \quad (18)$$

With equation (14) and (16) we can determine γ by

$$\frac{2\gamma}{3} - 2\gamma^2 = \frac{\gamma}{3} - 2\gamma^3.$$

This equation can be divided by 2γ , which leads to the quadratic equation

$$\gamma^2 - \gamma + \frac{1}{6} = 0.$$

The solution is given by

$$\gamma = \frac{1}{2} \pm \frac{\sqrt{3}}{6},$$

but only the solution $\gamma = \frac{1}{2} + \frac{\sqrt{3}}{6}$ yields an A-stable method (see [2]). From (18) it follows $b_3\beta_{32}\beta_2 = 0$ and from (14) we have $b_3\beta_{32}\alpha_2^2 \neq 0$. With (13) it follows that $\beta_2 = 0$ holds. From (15) and (17) we get

$$b_3\beta_{32}\alpha_2^3 = \gamma^2 - 3\gamma^3.$$

Using (14) we obtain $\alpha_2 = 3\gamma$. The variables a_{31} and a_{32} are free and can be chosen by $a_{31} = 0$ and $a_{32} = 1$. Then the remaining coefficients are given by

$$\begin{aligned} b_1 &= \frac{7}{18} - \frac{1}{18}\sqrt{3}, & b_2 &= \frac{1}{9} - \frac{1}{9}\sqrt{3}, & b_3 &= \frac{1}{2} + \frac{1}{6}\sqrt{3}, \\ \gamma_{31} &= \frac{7}{18} - \frac{7}{18}\sqrt{3}, & \gamma_{32} &= -\frac{8}{9} - \frac{1}{9}\sqrt{3}. \end{aligned}$$

For the embedded method we choose $\hat{b}_2 = 1/10$. The other two variables are determined by (A1) and (A2), i. e. by

$$\hat{b}_3 = \frac{1/2 - \gamma}{\beta_3} = \frac{1}{6}(3 + \sqrt{3}), \quad \hat{b}_1 = \frac{9}{10} - \hat{b}_3 = \frac{2}{5} - \frac{\sqrt{3}}{6}.$$

The coefficients of our new ROS3PR method are summarised in Table 1.

γ	=	7.8867513459481287e - 01		
α_{21}	=	2.3660254037844388e + 00	γ_{21}	= -2.3660254037844388e + 00
α_{31}	=	0.0000000000000000e + 00	γ_{31}	= -2.8468642516567449e - 01
α_{32}	=	1.0000000000000000e + 00	γ_{32}	= -1.0813389786187642e + 00
b_1	=	2.9266384402395124e - 01	\hat{b}_1	= 1.1132486540518712e - 01
b_2	=	-8.1338978618764143e - 02	\hat{b}_2	= 1.0000000000000001e - 01
b_3	=	7.8867513459481287e - 01	\hat{b}_3	= 7.8867513459481287e - 01

Table 1: Set of coefficients for ROS3PR.

3.2 The ROS3Pw method

The ROS3Pw method is an extension of ROS3P since it satisfies a further condition, i. e. condition (B2). As in the previous section the order conditions from Lubich and Ostermann [8] are replaced by the new order conditions (6) and (7) for $k = 3, 4$ and $l = 1, \dots, k - 2$. In the last section we saw that α_3 is a free variable. For our new method α_3 is determined by the additional

condition (B2). Altogether we have

$$\alpha_3 = 3 - \sqrt{3}, \quad b_1 = \frac{13}{36} + \frac{1}{12}\sqrt{3}, \quad b_2 = \frac{1}{3} - \frac{7}{27}\sqrt{3}, \quad b_3 = \frac{11}{36} + \frac{19}{108}\sqrt{3}.$$

The coefficients for the embedded method can be computed in the same way as for the ROS3PR method, i. e. we choose $\hat{b}_2 = 1/10$. In Table 2 we summarise the coefficients of our new ROS3PRw method.

γ	=	$7.8867513459481287e - 01$			
α_{21}	=	$2.3660254037844388e + 00$	γ_{21}	=	$-2.3660254037844388e + 00$
α_{31}	=	$5.0000000000000000e - 01$	γ_{31}	=	$-8.6791218280355165e - 01$
α_{32}	=	$7.6794919243112270e - 01$	γ_{32}	=	$-8.7306695894642317e - 01$
b_1	=	$5.0544867840851759e - 01$	\hat{b}_1	=	$2.8973180237214197e - 01$
b_2	=	$-1.1571687603637559e - 01$	\hat{b}_2	=	$1.0000000000000001e - 01$
b_3	=	$6.1026819762785800e - 01$	\hat{b}_3	=	$6.1026819762785800e - 01$

Table 2: Set of coefficients for ROS3PRw

3.3 The ROS3PL method

Next we consider the ROS3PL method from Lang and Teleaga [6]. The method has 4 internal stages, order 3 and is stiffly accurate, i. e. it holds

$$b_i = \beta_{si}, \quad i = 1, \dots, s \quad \text{and} \quad c_s = 1.$$

We consider the order conditions (A1), (A2), (A3a), (A3b) and (7) for $k = 3, 4$ and $l = 1, \dots, k-2$. Condition (6) is automatically satisfied since the method is stiffly accurate. Therefore we have the following equations

$$\begin{aligned} b_1 + b_2 + b_3 + b_4 &= 1, \\ b_2\beta_2 + b_3\beta_3 + b_4\beta_4 &= \frac{1}{2} - \gamma, \\ b_2\alpha_2^2 + b_3\alpha_3^2 + b_4\alpha_4^2 &= \frac{1}{3}, \\ b_3\beta_{32}\beta_2 + b_4\beta_{42}\beta_2 + b_4\beta_{43}\beta_3 &= \frac{1}{6} - \gamma + \gamma^2. \end{aligned}$$

Since the ROS3PL method is stiffly accurate the conditions simplify to

$$b_1 + b_2 + b_3 = 1 - \gamma, \quad (19)$$

$$b_2\beta_2 + b_3\beta_3 = \frac{1}{2} - 2\gamma + \gamma^2, \quad (20)$$

$$b_2\alpha_2^2 + b_3\alpha_3^2 = \frac{1}{3} - \gamma, \quad (21)$$

$$b_3\beta_{32}\beta_2 = \frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3. \quad (22)$$

The new order condition (7) simplifies to the following equations in the case $k = 3, 4$ and $l = 1, \dots, k - 2$

$$b_3\beta_{32}\alpha_2^2 = 2\gamma^3 - 2\gamma^2 + \frac{1}{3}\gamma, \quad (23)$$

$$b_3\beta_{32}\alpha_2^3 = 3\gamma^3 - \gamma^2 + \gamma(b_2\alpha_2^3 + b_3\alpha_3^3), \quad (24)$$

$$3b_3\beta_{32}\alpha_2^2 = 2\gamma^4 - 3\gamma^2 + \frac{2}{3}\gamma. \quad (25)$$

From (23) and (25) we get the non-linear equation

$$\gamma^3 - 3\gamma^2 + \frac{3}{2}\gamma - \frac{1}{6} = 0.$$

One solution of this equation is $\gamma \approx 0.43$. Then conditions (22) and (23) imply $\beta_2 = 0$. Next we simplify condition (24) to

$$b_2\alpha_2^3 + b_3\alpha_3^3 = 4\gamma^3 - 7\gamma^2 + \frac{5}{3}\gamma.$$

Variables α_2 and α_3 are free variables. We set $\alpha_2 = 1/2$ and $\alpha_3 = 1$. Then equations (21) and (24) simplify to

$$\begin{aligned} \frac{1}{8}b_2 + b_3 &= \frac{1}{6} - 2\gamma^2 \\ \frac{1}{4}b_2 + b_3 &= \frac{1}{3} - \gamma \end{aligned}$$

and we get

$$\begin{aligned} b_2 &= 16\gamma^2 - 8\gamma + \frac{4}{3}, \\ b_3 &= \gamma - 4\gamma^2. \end{aligned}$$

With condition (19) we get b_1 , i. e.

$$b_1 = -\frac{1}{3} + 6\gamma - 12\gamma^2.$$

Coefficient β_3 can be computed from equation (19), i. e.

$$\beta_3 = \frac{\frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3}{\gamma - 4\gamma^2}$$

and finally we have for the coefficient β_{32}

$$\beta_{32} = \frac{2\gamma^3 - 2\gamma^2 + \frac{1}{3}\gamma}{4\gamma - 16\gamma^2}.$$

For the remaining coefficients we chose $\alpha_{32} = \alpha_{41} = \alpha_{42} = 1/2$.

For the embedded method we have the conditions for ODEs up to order 2, i. e.

$$\begin{aligned}\hat{b}_1 + \hat{b}_2 + \hat{b}_3 + \hat{b}_4 &= 1, \\ \hat{b}_3\beta_3 + \hat{b}_4\beta_4 &= \frac{1}{2} - \gamma.\end{aligned}$$

For condition (7) in the case $k = 3$ and $l = 1$ we get

$$2\gamma^4 - \gamma^2(\hat{b}_2\alpha_2^2 + \hat{b}_3\alpha_3^2 + \hat{b}_4\alpha_4^2) + 2\gamma(\hat{b}_3\beta_{32}\alpha_2^2 + \hat{b}_4\beta_{42}\alpha_2^2 + \hat{b}_4\beta_{43}\alpha_3^2) - \hat{b}_4\beta_{43}\beta_{32}\alpha_2^2 = 0.$$

Moreover we want to satisfy the condition $R(\infty) = 1 - \hat{\mathbf{b}}^\top B^{-1} \mathbf{c} = r_\infty$. It follows

$$\gamma^4 - \gamma^3(\hat{b}_1 + \hat{b}_2 + \hat{b}_3 + \hat{b}_4) + \gamma^2(\hat{b}_3\beta_3 + \hat{b}_4\beta_4) - \gamma\hat{b}_4\beta_{43}\beta_3 = \gamma^4 r_\infty.$$

and

$$\gamma^4 - 2\gamma^3 + \frac{1}{2}\gamma^2 - \gamma\hat{b}_4 \left(\frac{1}{2} - 2\gamma + \gamma^2 \right) = \gamma^4 r_\infty.$$

Finally we obtain for \hat{b}_4

$$\hat{b}_4 = \frac{(1 - r_\infty)\gamma^3 - 2\gamma^2 + \frac{1}{2}\gamma}{\frac{1}{2} - 2\gamma + \gamma^2}.$$

An L-stable embedded method does not exist, since for $r_\infty = 0$ we get $\hat{b}_4 = \gamma = b_4$. In our case we choose $r_\infty = -1/4$ and $\hat{b}_1 = 1/2$. Then it follows

$$\hat{b}_3 = \frac{\frac{1}{2} - \gamma - \hat{b}_4(1 - \gamma)}{\beta_3},$$

$$\hat{b}_2 = 1 - \hat{b}_1 - \hat{b}_3 - \hat{b}_4.$$

The coefficients of the ROS3PRL method are displayed in Table 3.

γ	=	4.3586652150845900e - 01		
α_{21}	=	5.0000000000000000e - 01	γ_{21}	= -5.0000000000000000e - 01
α_{31}	=	5.0000000000000000e - 01	γ_{31}	= -7.9156480420464204e - 01
α_{32}	=	5.0000000000000000e - 01	γ_{32}	= 3.5244216792751432e - 01
α_{41}	=	5.0000000000000000e - 01	γ_{41}	= -4.9788969914518677e - 01
α_{42}	=	5.0000000000000000e - 01	γ_{42}	= 3.8607515441580453e - 01
α_{43}	=	0.0000000000000000e + 00	γ_{43}	= -3.2405197677907682e - 01
b_1	=	2.1103008548132443e - 03	\hat{b}_1	= 5.0000000000000000e - 01
b_2	=	8.8607515441580453e - 01	\hat{b}_2	= 3.8752422953298199e - 01
b_3	=	-3.2405197677907682e - 01	\hat{b}_3	= -2.0949226315045236e - 01
b_4	=	4.3586652150845900e - 01	\hat{b}_4	= 3.2196803361747034e - 01

Table 3: Set of coefficients for ROS3PRL

3.4 The RODASPR method

Our last method, RODASPR, is an improvement of the RODASP method from [18]. The RODASP method has 6 internal stages, is stiffly accurate, and its embedded method is stiffly accurate, too. We start our considerations with the order conditions for ODEs up to order 4. In the case of a stiffly accurate

method they simplify to

$$b_1 + b_2 + b_3 + b_4 + b_5 = 1 - \gamma, \quad (26)$$

$$b_2\beta_2 + b_3\beta_3 + b_4\beta_4 + b_5\beta_5 = \frac{1}{2} - 2\gamma + \gamma^2, \quad (27)$$

$$b_2\alpha_2^2 + b_3\alpha_3^2 + b_4\alpha_4^2 + b_5 = \frac{1}{3} - \gamma, \quad (28)$$

$$b_3\beta_{32}\beta_2 + b_4(\beta_{42}\beta_2 + \beta_{43}\beta_3) + b_5(\beta_{52}\beta_2 + \beta_{53}\beta_3 + \beta_{54}\beta_4) = \frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3, \quad (29)$$

$$b_2\alpha_2^3 + b_3\alpha_3^3 + b_4\alpha_4^3 + b_5 = \frac{1}{4} - \gamma, \quad (30)$$

$$b_3\alpha_3\alpha_{32}\beta_2 + b_4\alpha_4(\alpha_{42}\beta_2 + \alpha_{43}\beta_3) + b_5(\alpha_{52}\beta_2 + \alpha_{53}\beta_3 + \alpha_{54}\beta_4) = \frac{1}{8} - \frac{1}{3}\gamma, \quad (31)$$

$$b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) + b_5(\beta_{52}\alpha_2^2 + \beta_{53}\alpha_3^2 + \beta_{54}\alpha_4^2) = \frac{1}{12} - \frac{2}{3}\gamma + \gamma^2, \quad (32)$$

$$b_4\beta_{43}\beta_{32}\beta_2 + b_5\beta_{53}\beta_{32}\beta_2 + b_5\beta_{54}\beta_{42}\beta_2 + b_5\beta_{54}\beta_{43}\beta_3 = \frac{1}{24} - \frac{2}{3}\gamma + 3\gamma^2 - 4\gamma^3 + \gamma^4. \quad (33)$$

The order conditions for the embedded method are given by

$$\beta_{51} + \beta_{52} + \beta_{53} + \beta_{54} = 1 - \gamma, \quad (34)$$

$$\beta_{52}\beta_2 + \beta_{53}\beta_3 + \beta_{54}\beta_4 = \frac{1}{2} - 2\gamma + \gamma^2, \quad (35)$$

$$\beta_{52}\alpha_2^2 + \beta_{53}\alpha_3^2 + \beta_{54}\alpha_4^2 = \frac{1}{3} - \gamma, \quad (36)$$

$$\beta_{53}\beta_{32}\beta_2 + \beta_{54}(\beta_{42}\beta_2 + \beta_{43}\beta_3) = \frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3. \quad (37)$$

In the case of a stiffly accurate method the conditions (6) are satisfied for all k . Condition (7) should be satisfied for $k = 3, 4, 5$ and $l = 1, \dots, k-2$. Using the above equations condition (7) with $k = 3$ and $l = 1$ simplifies to

$$b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^2 - \gamma(b_4\beta_{43}\beta_{32}\alpha_2^2 + b_5\beta_{53}\beta_{32}\alpha_2^2 + b_5\beta_{54}\beta_{42}\alpha_2^2 + b_5\beta_{54}\beta_{43}\alpha_3^2) = 2\gamma^5 - 3\gamma^4 + \gamma^3 - \frac{1}{12}\gamma^2. \quad (38)$$

For $k = 4$ and $l = 2$ after some simplifications we get

$$\begin{aligned} 5b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^2 - 4\gamma(b_4\beta_{43}\beta_{32}\alpha_2^2 + b_5\beta_{53}\beta_{32}\alpha_2^2 + b_5\beta_{54}\beta_{42}\alpha_2^2 + b_5\beta_{54}\beta_{43}\alpha_3^2) \\ = 2\gamma^6 - 6\gamma^4 + \frac{5}{3}\gamma^3 - \frac{1}{4}\gamma^2. \end{aligned} \quad (39)$$

Next we can manipulate both equations and receive

$$b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^2 = 2\gamma^6 - 8\gamma^5 + 6\gamma^4 - \frac{4}{3}\gamma^3 + \frac{1}{12}\gamma^2, \quad (40)$$

$$\begin{aligned} b_4\beta_{43}\beta_{32}\alpha_2^2 + b_5\beta_{53}\beta_{32}\alpha_2^2 + b_5\beta_{54}\beta_{42}\alpha_2^2 + b_5\beta_{54}\beta_{43}\alpha_3^2 \\ = 2\gamma^5 - 10\gamma^4 + 9\gamma^3 - \frac{7}{3}\gamma^2 + \frac{1}{6}\gamma. \end{aligned} \quad (41)$$

For the condition (7) with $k = 5$ and $l = 3$ we obtain

$$b_5\beta_{54}\beta_{43}\beta_{32}\beta_2 = 0. \quad (42)$$

Equations (40) and (42) imply that $\beta_2 = 0$. Next we consider the equations with α^3 , i. e. condition (7) with $k = 4, l = 1, k = 5, l = 2$, and $k = 6$ and $l = 3$. We obtain

$$\begin{aligned} b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^3 - \gamma(b_4\beta_{43}\beta_{32}\alpha_2^3 + b_5\beta_{53}\beta_{32}\alpha_2^3 + b_5\beta_{54}\beta_{42}\alpha_2^3 + b_5\beta_{54}\beta_{43}\alpha_3^3) \\ + \gamma^2 [b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) + b_5(\beta_{52}\alpha_2^2 + \beta_{53}\alpha_3^2 + \beta_{54}\alpha_4^2)] \\ = 3\gamma^5 - 2\gamma^4 + \frac{1}{4}\gamma^3, \end{aligned} \quad (43)$$

$$\begin{aligned} 5b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^3 - 4\gamma(b_4\beta_{43}\beta_{32}\alpha_2^3 + b_5\beta_{53}\beta_{32}\alpha_2^3 + b_5\beta_{54}\beta_{42}\alpha_2^3 + b_5\beta_{54}\beta_{43}\alpha_3^3) \\ + 3\gamma^2 [b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) + b_5(\beta_{52}\alpha_2^2 + \beta_{53}\alpha_3^2 + \beta_{54}\alpha_4^2)] \\ = 6\gamma^6 - 3\gamma^4 + \frac{1}{2}\gamma^3, \end{aligned} \quad (44)$$

$$\begin{aligned} 15b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^3 - 10\gamma(b_4\beta_{43}\beta_{32}\alpha_2^3 + b_5\beta_{53}\beta_{32}\alpha_2^3 + b_5\beta_{54}\beta_{42}\alpha_2^3 + b_5\beta_{54}\beta_{43}\alpha_3^3) \\ + 6\gamma^2 [b_3\beta_{32}\alpha_2^2 + b_4(\beta_{42}\alpha_2^2 + \beta_{43}\alpha_3^2) + b_5(\beta_{52}\alpha_2^2 + \beta_{53}\alpha_3^2 + \beta_{54}\alpha_4^2)] \\ = 6\gamma^7 - 4\gamma^4 + \frac{3}{4}\gamma^3. \end{aligned} \quad (45)$$

Equation (43)– (45) can be broken down to

$$b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^3 = 6\gamma^7 - 24\gamma^6 + 18\gamma^5 - 4\gamma^4 + \frac{1}{4}\gamma^3, \quad (46)$$

$$\begin{aligned} & b_4\beta_{43}\beta_{32}\alpha_2^3 + b_5\beta_{53}\beta_{32}\alpha_2^3 + b_5\beta_{54}\beta_{42}\alpha_2^3 + b_5\beta_{54}\beta_{43}\alpha_3^3 \\ &= 12\gamma^6 - 54\gamma^5 + 45\gamma^4 - 11\gamma^3 + \frac{3}{4}\gamma^2, \end{aligned} \quad (47)$$

$$\begin{aligned} & b_3\beta_{32}\alpha_2^3 + b_4(\beta_{42}\alpha_2^3 + \beta_{43}\alpha_3^3) + b_5(\beta_{52}\alpha_2^3 + \beta_{53}\alpha_3^3 + \beta_{54}\alpha_4^3) \\ &= 6\gamma^5 - 30\gamma^4 + 30\gamma^3 - 9\gamma^2 + \frac{3}{4}\gamma. \end{aligned} \quad (48)$$

Dividing equation (46) by (40) yields $\alpha_2 = 3\gamma$ and dividing (32) by (37) gives us

$$b_5 = \frac{\frac{1}{24} - \frac{2}{3}\gamma + 3\gamma^2 - 4\gamma^3 + \gamma^4}{\frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3}.$$

Next we consider equations (32) and (40) (divided by $2\gamma^2$) and obtain

$$\beta_3 = \frac{9}{2}\beta_{32}. \quad (49)$$

From equation (40) we get

$$\begin{aligned} & (b_4\beta_{43}\beta_{32} + b_5\beta_{53}\beta_{32} + b_5\beta_{54}\beta_{42})\alpha_2^2 \\ &= 2\gamma^5 - 10\gamma^4 + 9\gamma^3 - \frac{7}{3}\gamma^2 + \frac{1}{6}\gamma - b_5\beta_{54}\beta_{43}\alpha_3^2. \end{aligned}$$

Inserting this result into (47) leads to

$$b_5\beta_{54}\beta_{43}\alpha_3^2(\alpha_3 - 3\gamma) = 6\gamma^2 \left[\gamma^4 - 4\gamma^3 + 3\gamma^2 - \frac{2}{3}\gamma + \frac{1}{24} \right].$$

Inserting the formula for b_5 yields

$$\beta_{54}\beta_{43}\alpha_3^2(\alpha_3 - 3\gamma) = 6\gamma^2 \left[\frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3 \right] = 6\gamma^2\beta_{54}\beta_{43}\beta_3,$$

where we use condition (37). Finally we get

$$\beta_3 = \frac{\alpha_3^2}{6\gamma^2}(\alpha_3 - 3\gamma).$$

Comparing (33) and (38) we see that

$$b_5\beta_{54}\beta_{43}\beta_3 = \frac{1}{24} - \frac{2}{3}\gamma + 3\gamma^2 - 4\gamma^3 + \gamma^4 = \frac{1}{2\gamma^2}b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^2$$

and it follows with $\alpha_2 = 3\gamma$ that $\beta_3 = \frac{9}{2}\beta_{32}$ holds. Dividing equation (37) by (33) and multiplying it by b_4 yields

$$b_4 \frac{\beta_{54}\beta_{43}\beta_3}{b_4\beta_{43}\beta_3} = b_4 \frac{\frac{1}{6} - \frac{3}{2}\gamma + 3\gamma^2 - \gamma^3}{\frac{1}{24} - \frac{2}{3}\gamma + 3\gamma^2 - 4\gamma^3 + \gamma^4} = \beta_{54}.$$

Moreover we need condition (43) for $k = 5$ and $l = 1$. After some simplifications we get

$$\begin{aligned} & b_5\beta_{54}\beta_{43}\beta_{32}\alpha_2^4 - \gamma(b_4\beta_{43}\beta_{32}\alpha_2^4 + b_5\beta_{53}\beta_{32}\alpha_2^4 + b_5\beta_{54}\beta_{42}\alpha_2^4 + b_5\beta_{54}\beta_{43}\alpha_3^4) \\ & + \gamma^2 [b_3\beta_{32}\alpha_2^4 + b_4(\beta_{42}\alpha_2^4 + \beta_{43}\alpha_3^4) + b_5(\beta_{52}\alpha_2^4 + \beta_{53}\alpha_3^4 + \beta_{54}\alpha_4^4)] \\ & - \gamma^3 [b_2\alpha_2^4 + b_3\alpha_3^4 + b_4\alpha_4^4 + b_5] = 4\gamma^5 - \gamma^4. \end{aligned} \quad (50)$$

In the next step we solve a system of non-linear equations to determine coefficients $b_2, b_3, b_4, \beta_{42}, \beta_{43}, \beta_{52}, \beta_{53}$, and β_{54} using the equations (27), (28), (29), (30), (32), (35), (36), and (50). Coefficients b_1 and α_{43} can be determined via (26) and (31). For determining α_{54} we use the further condition

$$\sum_{i=1}^4 \sum_{j=1}^i \alpha_{5i} \omega_{ij} = 1,$$

which is useful for DAEs of index 2, which are solved with inconsistent initial conditions (see [2] and [18]). After some simple manipulations this condition simplifies to

$$\alpha_{54}\beta_{43}\beta_3 = \frac{1}{2}\gamma - 2\gamma^2 + \gamma^3.$$

Coefficient α_{52} can be calculated with the help of the further condition [2]

$$\sum_{i=1}^{s-2} \sum_{j=1}^i \alpha_{s-1,i} \omega_{ij} \alpha_j^2 = 1,$$

where ω_{ij} are the entries of B^{-1} . This condition might be helpful if index-2 DAEs with inconsistent initial conditions are solved [2, 18]. The condition can be written as

$$\alpha_{52}\omega_{22}\alpha_2^2 + \alpha_{53}\omega_{32}\alpha_2^2 + \alpha_{53}\omega_{33}\alpha_3^2 + \alpha_{54}\omega_{42}\alpha_2^2 + \alpha_{54}\omega_{43}\alpha_3^2 + \alpha_{54}\omega_{44}\alpha_4^2 = 1$$

or as

$$(\alpha_{52}\gamma^2 - \gamma\alpha_{53}\beta_{32} + \alpha_{54}(\beta_{43}\beta_{32} - \gamma\beta_{42})\alpha_2^2 + (\alpha_{53}\gamma^2 - \gamma\alpha_{54}\beta_{43})\alpha_3^2 + \gamma^2\alpha_{54}\alpha_4^2 = \gamma^3.$$

Coefficients α_{32} and α_{43} can be calculated with the help of the condition for methods of order 6, i. e. with

$$\sum b_i \alpha_i^2 \alpha_{ij} \alpha_j^2 = \frac{1}{18}.$$

The coefficients of the RODASPR method are displayed in Table 4.

γ	=	2.5000000000000000e - 01		
α_{21}	=	7.5000000000000000e - 01	γ_{21}	= -7.5000000000000000e - 01
α_{31}	=	7.5162877593868457e - 02	γ_{31}	= -8.8644359075349941e - 02
α_{32}	=	2.4837122406131545e - 02	γ_{32}	= -2.8688974257983398e - 02
α_{41}	=	1.6532708886396510e + 00	γ_{41}	= -4.8470034585330284e + 00
α_{42}	=	2.1545706385445562e - 01	γ_{42}	= -3.1583244269672095e - 01
α_{43}	=	-1.3157488872766792e + 00	γ_{43}	= 4.9536568360123221e + 00
α_{51}	=	1.9385003738039885e + 01	γ_{51}	= -2.6769456904577400e + 01
α_{52}	=	1.2007117225835324e + 00	γ_{52}	= -1.5066459128852787e + 00
α_{53}	=	-1.9337924059522791e + 01	γ_{53}	= 2.7200131480460591e + 01
α_{54}	=	-2.4779140110062559e - 01	γ_{54}	= 8.2597133700208525e - 01
α_{61}	=	-7.3844531665375115e + 00	γ_{61}	= 6.5876206496361416e + 00
α_{62}	=	-3.0593419030174646e - 01	γ_{62}	= 3.6807059172993878e - 01
α_{63}	=	7.8622074209377981e + 00	γ_{63}	= -6.7423520694658121e + 00
α_{64}	=	5.7817993590145966e - 01	γ_{64}	= -1.0619631475741095e - 01
α_{65}	=	2.5000000000000000e - 01	γ_{65}	= -3.5714285714285715e - 01
b_1	=	-7.9683251690137014e - 01	\hat{b}_1	= -7.3844531665375115e + 00
b_2	=	6.2136401428192344e - 02	\hat{b}_2	= -3.0593419030174646e - 01
b_3	=	1.1198553514719862e + 00	\hat{b}_3	= 7.8622074209377981e + 00
b_4	=	4.7198362114404874e - 01	\hat{b}_4	= 5.7817993590145966e - 01
b_5	=	-1.0714285714285714e - 01	\hat{b}_5	= 2.5000000000000000e - 01
b_6	=	2.5000000000000000e - 01	\hat{b}_6	= 0.0000000000000000e + 00

Table 4: Set of coefficients for RODASPR

4 Numerical results

In this section we compare the new methods with the old ones. Furthermore we include the ROS34PRW method (see [12] and [13], which is an extension

of the ROS34PW2 method [15]. We list the most important properties of our methods in Table 5.

Table 5: Properties of the selected ROW methods

Name	s	p	$R(\infty)$	stiffly acc.	reference
ROS3P	3	3	0.73	no	[7]
ROS3P _w	3	3	0.73	no	[15]
ROS34PW2	4	3	0	yes	[15]
ROS3PL	4	3	0	yes	[6]
RODASP	6	4	0	yes	[18]
ROS3PR	3	3	0.73	no	Section 3.1
ROS3PR _w	3	3	0.73	no	Section 3.2
ROS34PRW	4	3	0	yes	[12]
ROS3PRL	4	3	0	yes	Section 3.3
RODASPR	6	4	0	yes	Section 3.4

4.1 Example of Prothero–Robinson

First we consider the well known example from Prothero and Robinson

$$\dot{u} = \lambda(u - \varphi(t)) + \dot{\varphi}(t), \quad u(0) = \varphi(0) \quad (51)$$

with

$$\varphi(t) = \sin t.$$

We solve the ODE (51) with equidistant step sizes $\tau = \frac{1}{10 \cdot 2^k}$, $k = 0, \dots, 13$ in the time interval $(0, 1/10]$. In Figure 1 we present the numerical results for $\lambda = -1$ (left) and $\lambda = -10^6$ (right). In the case $\lambda = -1$ all methods converge with order 3 or 4, as it is to be expected from the order of convergence. The other case $\lambda = -10^6$ shows that traditional methods like ROS3P, ROS3P_w, ROS3PL, ROS34PW2 and RODASP have order reduction. The methods satisfying the new order conditions show better convergence properties. In Table 4.1 we show the numerically observed order of convergence for all considered methods.

	τ	$\frac{1}{10}$	$\frac{1}{20}$	$\frac{1}{40}$	$\frac{1}{80}$	$\frac{1}{160}$
ROS3P	$\ \epsilon\ $	1.66e-09	3.05e-10	7.14e-11	1.66e-11	3.98e-12
	q_{num}		2.45	2.09	2.10	2.06
ROS3PR	$\ \epsilon\ $	4.96e-12	3.80e-13	3.86e-14	4.72e-15	5.00e-16
	q_{num}		3.71	3.30	3.03	3.24
ROS3Pw	$\ \epsilon\ $	4.80e-05	4.40e-06	5.16e-07	6.00e-08	7.18e-09
	q_{num}		3.45	3.09	3.10	3.06
ROS3PRw	$\ \epsilon\ $	1.41e-07	5.23e-09	2.63e-10	1.60e-11	8.38e-13
	q_{num}		4.75	4.31	4.04	4.25
ROS34PW2	$\ \epsilon\ $	5.85e-10	1.46e-10	3.66e-11	9.15e-12	2.29e-12
	q_{num}		2.00	2.00	2.00	2.00
ROS34PR	$\ \epsilon\ $	8.00e-14	1.39e-14	4.22e-15	1.83e-15	8.77e-16
	q_{num}		2.53	1.72	1.20	1.06
ROS3PL	$\ \epsilon\ $	2.39e-10	5.99e-11	1.50e-11	3.75e-12	9.39e-13
	q_{num}		2.00	2.00	2.00	2.00
ROS3PRL	$\ \epsilon\ $	1.02e-12	1.34e-13	1.34e-14	1.61e-15	1.36e-15
	q_{num}		2.92	3.32	3.06	0.24
RODASP	$\ \epsilon\ $	3.38e-13	2.98e-14	2.95e-15	3.44e-16	3.12e-17
	q_{num}		3.50	3.34	3.10	
RODAS3PR	$\ \epsilon\ $	3.04e-13	1.90e-14	1.19e-15	7.59e-17	7.04e-18
	q_{num}		4.00	4.00		

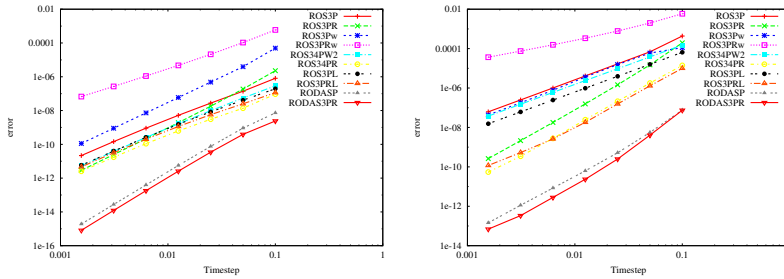


Figure 2: τ versus error for (52) velocity u (left) and pressure p (right)

as expected. In the case of the pressure component it can be observed that the new methods provide more accurate results than the older ones, since the older methods do not satisfy the new order conditions from [13].

Conclusions and outlook

In this note we consider traditional ROW methods like ROS3P, ROS3Pw, ROS3PL, ROS34PW2, and RODASP and equip these methods with further order conditions from [13]. The number of stages does not change, but these new methods give more accurate results than the old ones. In the next step these methods should be tested on more realistic problems.

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